

Twisted Order Parameter applied to Dimerized Ladders

J. Almeida*, M.A. Martin-Delgado* and G. Sierra*

**Departamento de Física Teórica I, Universidad Complutense. 28040 Madrid, Spain.*

**Instituto de Física Teórica, C.S.I.C.- U.A.M., Madrid, Spain.*

We apply the twisted order parameter (TOP) for dimerized quantum spin ladders to locate the critical phases that separate gapped phases representing quantum spin liquids of various types. Using the DMRG, method we find that the TOP is a good order parameter for these systems regardless the number of legs. As a check, we reproduce with DMRG and periodic boundary conditions the computations previously done with Quantum Montecarlo for one-dimensional $S=1/2$, $S=1$, $S=3/2$ and $S=2$ Heisenberg chains with alternating bonds.

PACS numbers: 75.10.Jm 75.10.-b 74.20.Mn

I. INTRODUCTION

The physics of quantum spin ladders with dimerization [1] is an emblematic example of quantum phase transitions with a rich structure of both gapless and gapped phases [2, 4, 35]. The main issue in their quantum phase diagrams is to determine the location of critical points or lines, which typically separate massive phases. These phases exhibit quite strongly correlated properties like Haldane phases [5], an example of quantum spin liquid of great interest in condensed matter systems. Analytical methods have been applied to uncover this rich phase structure, some of them non-perturbative [1, 6, 7, 8, 9]. However, they are not sufficient to study with enough precision the whole range of coupling parameters entering in their quantum lattice Hamiltonians and, consequently, they have to be complemented with numerical studies [10, 11, 12, 13], which sometimes modify the conclusions achieved with analytical methods, either quantitative and/or qualitatively.

Quantum spin ladder systems are not mere theoretical constructs, but they have been experimentally synthesized in several types of materials [14, 15, 16, 18, 19], some of them as interesting as the superconducting cuprates compounds or another classes of materials which allow for not only antiferromagnetic couplings but also for ferromagnetic ones as we shall be considering in this work. Ladder systems are also valuable candidates to implement their physics in simulable optical lattices [20, 21], where the coupling constants of the models could be externally manipulated more easily than with standard materials. Furthermore, quantum spin chains and ladders have played a central role for ground test numerical simulations when the density matrix renormalization group (DMRG) was introduced [22, 23, 24, 25, 26].

A diversity of variants of quantum spin liquids appear as gapped phases in these dimerized spin ladders. These types of spin orders have been initially classified resorting to the string order parameter (SOP) [27, 28]. However, this initial SOP parameter was only valid for systems with spin magnitude $S = 1$. Then, a generalization valid for both integer and half-integer spin systems was introduced [29] and recently, we have been able to check their

validity in a large class of dimerized spin ladders [13] and we have found that the generalized SOP serves as a good order parameter to distinguish the many quantum phases appearing in those ladders when their number of legs and spin couplings are varied.

When moving from one gapped phase to another, this process generically implies crossing a critical point or line. Although the SOP parameter can detect the change associated to this phase crossing, however it does not perform so well when trying to locate the position of those critical points. To this end, another order parameter called twisted order parameter (TOP) has been introduced for spin chains [30] and some ladders [31, 32]. The TOP being non-local, it can be considered as a close relative of the SOP. In fact, we shall see that they play complementary roles: the SOP is better suited for classifying quantum spin liquids, whereas the TOP is more appropriate for finding their critical points.

The idea behind the TOP comes from the twist operator introduced in the proof of the Lieb-Schulz-Mattis theorem (LSM) [33, 34] in one-dimensional quantum spin systems. Under certain circumstances, namely, for half-integer S -spin chains, the system is proved to be gapless by creating a sort of twisted excited state along the chain, whose energy gap with respect to the ground state vanishes in the thermodynamic limit as $1/N$, where N is the length of the chain. Although this twist operator cannot be conclusive for the case of integer S -spin chains, thereby opening the door for the celebrated Haldane conjecture [5], it turns out that it can be used to locate the critical points of dimerized chains of arbitrary spins, either integer or half-integer. The way to see this connection is by means of the valence bond solid (VBS) states used as trial wavefunctions to qualitatively represent those gapped quantum phases.

The existence of extensions of the LSM theorem for spin ladders [35] can also be used as a hint to trying to extend the notion of the TOP parameter to more complicated lattices beyond one-dimensional systems. For spin ladders with $S = \frac{1}{2}$ spins, this generalized LSM theorem only works for an odd number of legs. Interestingly enough, we have found that the generalized TOP parameter works for locating the critical points, regardless of the number of legs.

This paper is organized as follows: in Sect.II we introduce a set of quantum lattice Hamiltonians for spin ladders which present two different patterns of dimerization, either staggered or columnar, as well as antiferromagnetic or ferromagnetic couplings between their legs (chains); in Sect.III we present our numerical results for the TOP parameter measured in those dimerized spin ladders using DMRG calculations. With this information we can plot the TOP vs. the dimerization strength and detect critical points by the vanishing of the TOP parameter. Upon varying the dimerization patterns and the ferro- or antiferro-types of rung couplings, the number of zeros and shape of the TOP also changes in characteristic forms that serve us to distinguish among the set of quantum ladder Hamiltonians introduced in the previous section. Sect.IV is devoted to conclusions.

II. MODELS OF DIMERIZED SPIN LADDERS

In this paper we study quantum spin ladders that can be viewed as a certain number of bond-alternated Heisenberg chains stacked one on top of another and coupled between them via a coupling constant J' corresponding to a Heisenberg-like spin interaction. The bond alternation between neighbor spins on the same leg is such that every strong bond is followed by a weaker one. Every leg can then begin either with a strong or weak coupling, and that initial choice determines the dimerization pattern all the way through the ladder.

Then, to characterize completely our ladders we have to specify some parameters: the number of legs n_l , the ferromagnetic $J' < 0$ or antiferromagnetic $J' > 0$ nature of the Heisenberg coupling between legs and the dimerization pattern of every leg, given by the coupling constant γ .

The Hamiltonian that gives raise to this general set of families of dimerized Heisenberg ladders is:

$$H^{\text{OBC}} = \sum_{\ell} \sum_i J_{i,\ell} \mathbf{S}_i(\ell) \cdot \mathbf{S}_{i+1}(\ell) + J' \sum_{\ell,i} \mathbf{S}_i(\ell) \cdot \mathbf{S}_i(\ell+1) \quad (1)$$

where $\mathbf{S}_i(\ell)$ denotes a $S = 1/2$ spin operator at the site i in the leg ℓ , with $i = 1 \dots N$ and $\ell = 1 \dots n_l$. The set of couplings denoted by $J_{i,\ell}$ endows the ladders with certain dimerization patterns to be specified below.

We shall focus our attention on two and three leg ladders, in addition to spin chains. These cases will suffice to clarify the behavior of the TOP parameter under diverse dimerization patterns. Moreover, among the different possibilities of establishing a dimerization pattern on every leg, we will only be interested in two particular arrangements of bonds. We will denote the *staggered* dimerization pattern that with a $J_{i,\ell}$ distribution of the form $J_{i,\ell} = 1 + (-1)^{i+\ell}\gamma$ while the *columnar* pattern has a distribution $J_{i,\ell} = 1 - (-1)^i\gamma$, i.e., all the legs begin with a strong bond. In both cases the parameter γ is constrained to be within $-1 \leq \gamma \leq 1$.

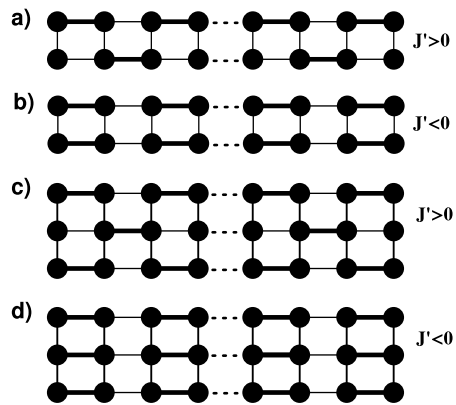


FIG. 1: Different dimerization patterns in two and three legs spin ladders: a) and c) are staggered, b) and d) are columnar. Thicker lines correspond to a coupling constant $J_{i,\ell} = 1 + \gamma$ and thinner ones to $J_{i,\ell} = 1 - \gamma$

We will also be interested in using not only open boundary conditions but also periodic ones. In this case, we have to modify the Hamiltonian (1) to take into account the interactions between both ends:

$$H^{\text{PBC}} = H^{\text{OBC}} + \sum_{\ell} J_{N,\ell} \mathbf{S}_N(\ell) \cdot \mathbf{S}_1(\ell) \quad (2)$$

Eq. (1) is not translationally invariant. On the contrary, if we consider ladders with an even number (greater than two) of sites per leg and using periodic boundary conditions, the Hamiltonian (2) is invariant under translations of the form $\mathbf{S}_i(\ell) \rightarrow \mathbf{S}_{i+2}(\ell)$ and also under reversal of the dimerization strength $\gamma \leftrightarrow -\gamma$.

The number of possible combinations of those ingredients described above is still high, and not all of them may have critical properties. This fact will depend essentially on the staggering pattern and coupling constant J' . In particular, for ladders with two and three legs, the models that may have critical phases for certain configurations of the microscopic parameters are the following ones: i/ the staggered antiferromagnetic two leg ladder, ii/ the columnar ferromagnetic two leg ladder, iii/ the staggered antiferromagnetic three leg ladder and iv/ the columnar ferromagnetic three leg ladder. These models are depicted in fig. 1.

III. RESULTS

Much like the string order parameter (SOP), the TOP is a non-local parameter since it involves non-local measurements. However, unlike the SOP, the success of the TOP relies in the 2π twist carried out between both ends of the system. This fact makes it unclear how will the DMRG perform when measuring it. This is in sharp contrast with the SOP case, which can be accurately measured using only a representative subsystem within the bulk of the whole system.

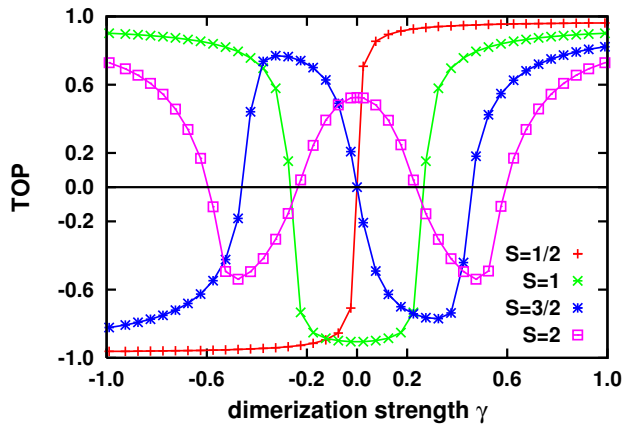


FIG. 2: DMRG computation of TOP for different one dimensional Heisenberg chains with alternated bonds. The size of the chains is $L = 64$ and periodic boundary conditions have been used.

A. Spin Chains

Due to this uncertainty and as a first check, we have reproduced the Quantum Montecarlo results for one dimensional dimerized chains [30] using DMRG-adapted methods. Fig. 2 shows the TOP computed for these chains using periodic boundary conditions. To compute these values the number of DMRG sweeps was set to three, the number of retained states of the density matrix was $m = 200$ and the Lanczos tolerance equal to 10^{-10} . With these parameters, the results obtained using DMRG and Quantum Montecarlo agree almost identically. In order to go a bit further and obtain better estimates of the critical points using DMRG, it is more convenient to use open ladders. Fig. 3 represents the TOP computed using open boundary conditions and different sizes of the chains. The largest size $L = 150$ was computed performing four DMRG sweeps, $m = 300$ and the tolerance equal to 10^{-9} , the less demanding case $L = 80$ required two sweeps, $m = 120$ and the tolerance equal to 10^{-8} . The critical points of each chain are those where the TOP is zero. Looking at the different graphs two observations are in order: on one hand we see that the location of the critical points is overestimated in the case of periodic boundary conditions compared to the case of open chains. On the other hand, the values of the critical points computed with open boundary conditions are in good agreement with the values of these points computed in the thermodynamic limit in other works [30]. In fact, from fig. 3 and the curves with $L = 150$ we see that for the $S = 1$ chain we obtain $\gamma_c = 0.254$, for $S = 3/2$ $\gamma_c = 0.426$. The case with $S = 2$ has two critical points at $\gamma_c = 0.184$ and $\gamma_c = 0.522$. These values can be respectively compared with the previously computed $\gamma_c = 0.25997(3)$, $\gamma_c = 0.43131(7)$, $\gamma_c = 0.1866(7)$, $0.5500(1)$.

Regarding the critical points $\gamma_c = 0$ in cases with

$S = 1/2$ and $S = 3/2$, we observe that the TOP unambiguously goes to zero using periodic boundary conditions. With open boundary conditions, however, the TOP is still far from zero even with $L = 150$, although the tendency is clearly to vanish as we increase the size. Interestingly enough, a similar slow converging behaviour precisely at $\gamma_c = 0$ has been also observed in [13] measuring the string order parameter.

B. Spin Ladders

In the rest of this section we will measure the TOP in the models described previously in Sect. II in order to test whether or not it can also be successfully applied to non strictly one dimensional cases.

We commented in the case of the spin chains that the TOP using open boundary conditions converged very slowly to zero at $\gamma_c = 0$ in those models that in fact possessed such a critical point. Since some of the ladders that we will study in this section have indeed a critical point close to $\gamma = 0$ we will use periodic boundary conditions to avoid the slow convergence of these points. Moreover, as we commented before, with periodic boundary conditions our models are invariant under sign reversal of the dimerization strength. This means that for a given computed critical point, say γ_c , there must exist another one equal to $-\gamma_c$. The difference in the value of these opposite points will then give us a hint about the truncation error of our DMRG computations.

The natural extension of the TOP as defined in [30] to systems with many legs is as follows:

$$z_\ell^1 := \langle \psi_0 | \exp \left\{ \frac{2\pi i}{N} \sum_{j=1}^N j S_j^z \right\} | \psi_0 \rangle \quad (3)$$

Where each operator now includes the contribution coming from each leg of the ladder $S_i = \sum_\ell S_i(\ell)$.

In fig. 4 we have computed the TOP on each one of the critical ladders described in the previous section. To run the DMRG we have set $m = 340$, the tolerance equal to 10^{-9} and performed three sweeps. For each one of the ladders we have used an arbitrary value of the constant J' . The critical lines of these models have been obtained by other techniques in references [10, 12, 13]. Since we are using periodic boundary conditions we are constrained to use smaller sizes than those considered in the references and hence no exact agreement is expected. With this consideration in mind, the location of the critical points in fig. 4, that is, the points where the TOP is zero, is in good agreement with those of the references, as comes out from table I.

The sign of the TOP is related with the nature of the VBS phase. From its definition it can be seen that its sign is given by a factor $(-1)^k$, where k is the number of isolated spins at the end of the chain. More explicitly, in

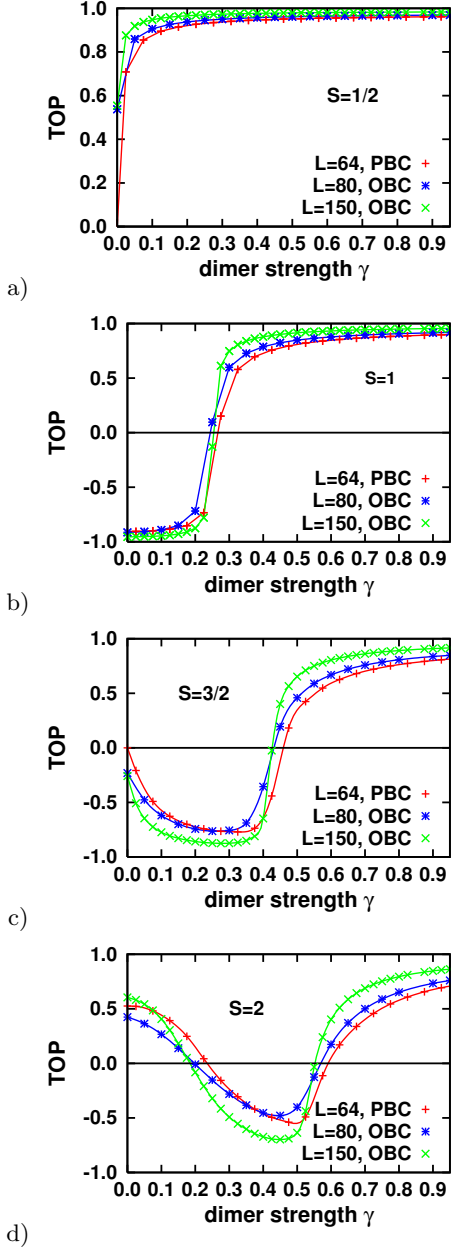


FIG. 3: TOP computed in various Heisenberg chains with alternated bonds and different spin values: a) $S = 1/2$, b) $S = 1$, c) $S = 3/2$, d) $S = 2$. Computations using open boundary conditions properly capture the location of the critical points as we increase the size of the system, however the convergence of the TOP towards zero at the particular point $\gamma_c = 0$ in the graphs a) and c) is very slow and makes a difference between both types of boundary conditions.

a general (m, n) -VBS state, $k = m$ if the number of sites is odd and $k = n$ if it is even.

We see in fig. 4 that the sign of the TOP is coherent with the VBS phases of each ladder. That is, in the cases of the two and three leg ladders with columnar dimerization the TOP is negative from $\gamma = 0$ up to the corresponding crit-

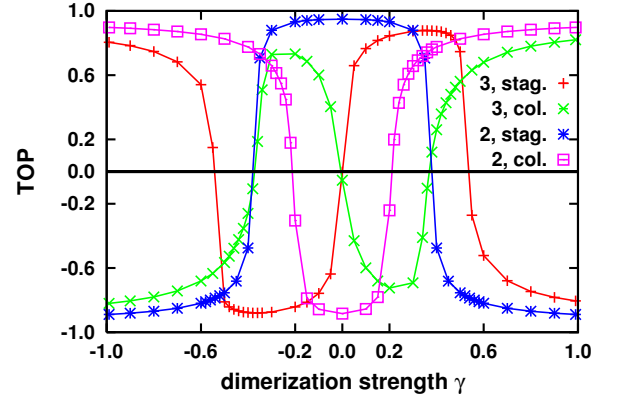


FIG. 4: TOP computed in ladders with columnar and staggered dimerization. The constant J' has a fixed value equal to $J' = -5$ in the two and three leg ladder with columnar dimerization and $J' = 1$ in the two and three leg with staggered dimerization. Boundary conditions have been used. The size of the two leg ladders is $L = 2 \times 60$, and $L = 3 \times 60$ for the three leg ladders

Ladder	J'	TOP	Other
3, stag.	1.0	$\gamma_c = 0.001, -0.542, 0.536$	$\gamma_c = 0, \pm 0.527$
3, col.	-5.0	$\gamma_c = 0.005, -0.372, 0.368$	$\gamma_c = 0, \pm 0.335$
2, stag.	1.0	$\gamma_c = -0.38, 0.38$	$\gamma_c = \pm 0.34$
2, col.	-5.0	$\gamma_c = -0.212, 0.211$	$\gamma_c = \pm 0.196$

TABLE I: Location of some critical points of different dimerized ladders. The identification of each ladder is done by means of the number of legs: two or three, and the dimerization pattern: staggered or columnar. We provide the values obtained with the TOP and the corresponding ones computed using different techniques. References related to these last values are given in the text.

ical values γ_c where the TOP is zero, and then the TOP is positive all the way to $\gamma = 1$. On the other hand the behavior of the TOP with the two and three leg ladders with staggered dimerization is the contrary. Since our computations have been all done using an even number of sites per leg, the sign of the TOP agrees with the characterization of the phases of each model done by means of the generalized SOP in refs. [12, 13]. That is, moving from $\gamma = 0$ to $\gamma = 1$ the two leg ladder with columnar dimerization moves from a $(1, 1)$ -VBS to a $(2, 0)$ -VBS while the three leg ladder with columnar dimerization moves from a $(2, 1)$ -VBS to a $(3, 0)$ -VBS. In these cases $k = 1$ and the sign of the TOP is negative in the first phases, and $k = 0$ and the sign of the TOP is positive in the second phases. In the case of the three leg ladder with staggered dimerization we move from a $(1, 2)$ -VBS to a $(2, 1)$ -VBS and again the sign of the TOP is correct according to the value of k . We have no information on the VBS phases of the two leg ladder with staggered dimer-

ization but in this particular case the only possibility to obtain a negative value of the TOP is a (1, 1)-VBS, while a positive TOP could be a (2, 0)-VBS or a (0, 2)-VBS.

IV. CONCLUSIONS

The results shown in the previous section reveal that the DMRG algorithm is well suited to compute the twisted order parameter even with open boundary conditions. We have applied TOP parameter to four different spin ladder systems and estimated the location of their critical points. We find agreement with other DMRG calculations which compute the vanishing of the gap directly. We have checked that the TOP computation is not only restricted to strictly one dimensional systems

but it also works in two- and three-leg ladders. This holds true despite the LSM theorem based on the twist operator only works for ladders with an odd number of legs and $S = \frac{1}{2}$ spins. In this sense, the twisted order parameter serves as a suitable and complementary tool to the string order parameter in the characterization of quantum phases in dimerized spin systems.

Acknowledgements: Part of the computations of this work were performed with the High Capacity Computational Cluster for Physics of UCM (HC3PHYS UCM), funded in part by UCM and in part with FEDER funds. We acknowledge financial support from DGS grants under contracts BFM 2003-05316-C02-01, FIS2006-04885, and the ESF Science Programme INSTANS 2005-2010.

-
- [1] M. A. Martin-Delgado, R. Shankar and G. Sierra, "Phase Transitions in Staggered Spin Ladders"; Phys. Rev. Lett. **77**, 3443 (1996).
 - [2] I. Affleck, F. D. M. Haldane, "Critical theory of quantum spin chains"; Phys. Rev. **B** 36 (1987) 5291.
 - [35] I. Affleck, Les Houches 1988-Session XLIX: *Fields, strings and critical phenomena* (North-Holland, Amsterdam 1990), chap. Field Theory Methods and Quantum Critical Phenomena, pp. 563-640.
 - [4] *Strongly Correlated Magnetic and Superconducting Systems*, Lecture Notes in Physics, Proceedings of the El Escorial Summer School 1996. Eds. G. Sierra and M. A. Martin-Delgado Springer-Verlag (1997).
 - [5] F. D. M. Haldane, "Continuum dynamics of the 1-D Heisenberg antiferromagnet: Identification with the O(3) nonlinear sigma model", Phys. Lett. **A** 93, 464-468 (1982).
 - [6] V. N. Kotov, J. Oitmaa and Zheng Weihong; "Excitation spectrum and ground-state properties of the S=1/2 Heisenberg ladder with staggered dimerization" Phys. Rev. **B** **59**, 11377 - 11383 (1999).
 - [7] Y.-J. Wang and A. A. Nersisyan, "Ising model description of the SU(2)₁ quantum critical point in a dimerized two-leg spin-1/2 ladder" Nucl. Phys. **B** 583, 671 (2000).
 - [8] M. Azzouz, K. Shahin, G.Y. Chitov, "Spin-Peierls instability in the spin- 1/2 Heisenberg three-leg ladder"; Phys. Rev. **B** 76, 132410 (2007).
 - [9] G.Y. Chitov, B. Ramakko, M. Azzouz; "Quantum Criticality in Dimerized Spin Ladders", arXiv0709.3256C.
 - [10] M. A. Martin-Delgado, J. Dukelsky and G. Sierra, "Phase diagram of the 2-leg Heisenberg ladder with alternating dimerization". Phys. Lett. **A** 250, 87 (1998).
 - [11] K. Okamoto, "Phase diagram of the S=1/2 two-leg spin ladder with staggered bond alternation" Phys. Rev. **B** 67, 212408 (2003).
 - [12] J. Almeida, M.A. Martin-Delgado, G. Sierra, "DMRG study of the Bond Alternating S=1/2 Heisenberg ladder with Ferro-Antiferromagnetic couplings". Phys. Rev. **B** **76**, 184428 (2007).
 - [13] J. Almeida, M.A. Martin-Delgado, G. Sierra, "Critical lines and massive phases in quantum spin ladders with dimerization"; arXiv:0707.4452 (2007)
 - [14] E. Dagotto, T. M. Rice, "Surprises on the Way from One- to Two-Dimensional Quantum Magnets: The Ladder Materials", Science **271** 618 - 623, (1996).
 - [15] E. Dagotto, Rep. Prog. Phys. **62** 1525-1571. "Experiments on ladders reveal a complex interplay between a spin-gapped normal state and superconductivity",
 - [16] Z. Hiroi, M. Azuma, M. Takano and Y. Bando, J. Sol. State Chem. 95, 230 (1991).
 - [17] M. Azuma, Z. Hiroi, M. Takano, K. Ishida and Y. Kitaoka, Phys. Rev. Lett. **73**, 3463 (1994).
 - [18] B. Batlogg et al., Bull. Am. Phys. Soc. 40, 327 (1995).
 - [19] Y. Hosokoshi et al., Phys. Rev. **B** 60, 12924-12932 (1999).
 - [20] M. Greiner, O. Mandel, T. Esslinger, Th. W. Hänsch, and I. Bloch, Nature **415**, 39 (2002); M. Greiner, O. Mandel, Th. W. Hänsch, and I. Bloch, Nature **419**, 51 (2002)
 - [21] J. J. Garcia-Ripoll, M. A. Martin-Delgado, J. I. Cirac, "Implementation of Spin Hamiltonians in Optical Lattices"; Phys. Rev. Lett. **93**, 250405 (2004); cond-mat/0404566.
 - [22] S.R. White, "Density-matrix algorithms for quantum renormalization groups"; Phys. Rev. Lett. **69**, 2863 (1992).
 - [23] S.R. White, Phys. Rev. **B** **48**, 10345 (1993)
 - [24] K. Hallberg, "New Trends in Density Matrix Renormalization"; Adv.Phys. **55** 477-526 (2006); cond-mat/0609039.
 - [25] A. Schollwöck, *The density matrix renormalization group*, Rev. Mod. Phys., **77**, 259 (2005).
 - [26] *Density Matrix Renormalization*, edited by I. Peschel, X. Wang, M. Kaulke and K. Hallberg (Series: Lecture Notes in Physics, Springer, Berlin, 1999)
 - [27] M. den Nijs, K. Rommelse, "Preroughening transitions in crystal surfaces and valence-bond phases in quantum spin chains", Phys. Rev. **B** **40**, 4709 (1989).
 - [28] T. Kennedy, H. Tasaki, "Hidden $Z_2 \times Z_2$ symmetry breaking in Haldane-gap antiferromagnets", Phys. Rev. **B** **45**, 304 (1992).
 - [29] M. Oshikawa, "Hidden $Z_2 \times Z_2$ symmetry in quantum spin chains with arbitrary integer spin"; 3. Phys.: Condens. Matter **4** 7469-7488 (1992).
 - [30] M. Nakamura, S. Todo, "Order parameter to characterize Valence-Bond solid states in quantum spin chains". Phys.

- Rev. Lett. **89**, 77204 (2002).
- [31] M. Nakamura, S. Todo, “Novel Order Parameter to Characterize Valence-Bond-Solid States”. Prog. Theor. Phys. Supplement, **145**, 217-220 (2002); arXiv:cond-mat/0201204.
 - [32] M. Matsumoto, T. Sakai, M. Sato, H. Takayama, S. Todo, “Quantum phase transitions of spin chiral nanotubes”; Physica **E** 29, 660 (2005); arXiv:cond-mat/0506626).
 - [33] E. Lieb, T. Schultz, and D. Mattis, “Two soluble models of an antiferromagnetic chain”, Ann. Phys. (N.Y.) **16**, 407-466 (1961).
 - [34] I. Affleck and E.H. Lieb, “A proof of part of Haldane’s conjecture on quantum spin chains”, Lett. Math. Phys. **12**, 57-69 (1986).
 - [35] I. Affleck, “Spin gap and symmetry breaking in CuO_2 layers and other antiferromagnets”, Phys. Rev. **B** 37, 5186 - 5192 (1988).